Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1805jxb

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	INPADOC: New family current-awareness alert (SDI) available
NEWS	4	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	5	SEP 01	New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS	6	SEP 27	STANDARDS will no longer be available on STN
NEWS	7	SEP 27	SWETSCAN will no longer be available on STN
NEWS	8	OCT 28	KOREAPAT now available on STN
NEWS	9	NOV 18	Current-awareness alerts, saved answer sets, and current search transcripts to be affected by CERAB, COMPUAB, ELCOM, and SOLIDSTATE reloads
NEWS	10	NOV 30	PHAR reloaded with additional data
NEWS	11	DEC 01	LISA now available on STN

NEWS EXPRESS	OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 11:09:45 ON 03 DEC 2004

=> file .pub

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'MEDLINE' ENTERED AT 11:10:10 ON 03 DEC 2004

FILE 'BIOSIS' ENTERED AT 11:10:10 ON 03 DEC 2004
Copyright (c) 2004 The Thomson Corporation.

=> s ekins s/au
L1 29 EKINS S/AU

```
=> e ekins s/au
E1            3     EKINS ROGER P/AU
E2            1     EKINS ROGER PHILIP/AU
E3           29 --> EKINS S/AU
E4           66     EKINS SEAN/AU
E5            2     EKINS W L/AU
E6            1     EKINTUMAS D/AU
E7            1     EKIRIWANG JAMES T/AU
E8           10     EKIS G/AU
E9            2     EKIS IMANTS/AU
E10           6     EKIS M/AU
E11           1     EKIS M L/AU
E12           4     EKISA E G/AU

=> s e3-4
L2           95 ("EKINS S"/AU OR "EKINS SEAN"/AU)

=> s l2 and 3d/4d-qsar and cyp2d6
'4D-QSAR' IS NOT A VALID FIELD CODE
'4D-QSAR' IS NOT A VALID FIELD CODE
L3            0 L2 AND 3D/4D-QSAR AND CYP2D6

=> s l2 and cyp2d6
L4           15 L2 AND CYP2D6

=> s l4 and (four dimensional)
L5            2 L4 AND (FOUR DIMENSIONAL)

=> d 1-2 bib ab

L5   ANSWER 1 OF 2     MEDLINE on STN
AN   2000242567     MEDLINE
DN   PubMed ID: 10780267
TI   Three and four dimensional-quantitative structure
     activity relationship (3D/4D-QSAR) analyses of CYP2D6
     inhibitors.
AU   Ekins S; Bravi G; Binkley S; Gillespie J S; Ring B J; Wikel J H;
     Wrighton S A
CS   Department of Drug Disposition, Lilly Research Laboratories, Eli Lilly and
     Co., Lilly Corporate Center, Indianapolis, IN 46285, USA.
SO   Pharmacogenetics, (1999 Aug) 9 (4) 477-89.
     Journal code: 9211735. ISSN: 0960-314X.
CY   ENGLAND: United Kingdom
DT   Journal; Article; (JOURNAL ARTICLE)
LA   English
FS   Priority Journals
EM   200005
ED   Entered STN: 20000525
     Last Updated on STN: 20000525
     Entered Medline: 20000512
AB   Three- and four-dimensional quantitative structure
     activity relationship (3D/4D-QSAR) pharmacophore models of competitive
     inhibitors of CYP2D6 were constructed using data from our
     laboratory or the literature.  The 3D-QSAR pharmacophore models of the
     common structural features of CYP2D6 inhibitors were built using
     the program Catalyst (Molecular Simulations, San Diego, CA, USA).  These
     3D-QSAR models were compared with 3D and 4D-QSAR partial least squares
     (PLS) models which were constructed using molecular surface-weighted
     holistic invariant molecular (MS-WHIM) descriptors of size and shape of
     inhibitors.  The first Catalyst model was generated from multiple
     conformers of competitive inhibitors (n = 20) of CYP2D6 mediated
     bufurolol 1'-hydroxylation.  This model demonstrated a correlation of
     observed and predicted Ki (apparent) values of r = 0.75.  A second
     Catalyst model was constructed from literature derived Ki (apparent)
```

values (n = 31) for the inhibition of **CYP2D6**. This model provided a correlation of observed and predicted inhibition for **CYP2D6** of r = 0.91. Both Catalyst Ki pharmacophores were then validated by predicting the Ki (apparent) of a test set of known **CYP2D6** inhibitors (n = 15). Ten out of 15 of these Ki (apparent) values were predicted to be within one log residual of the observed value using our **CYP2D6** inhibitor model, while the literature model predicted nine out of 15 values. Similarly, 3D- and 4D-QSARs derived from PLS MS-WHIM for our dataset yielded predictable models as assessed using cross-validation. The corresponding cross-validated PLS MS-WHIM model for the literature dataset yielded a comparable 3D-QSAR and improved 4D-QSAR value. Such computational models will aid in future prediction of drug-drug interactions.

L5 ANSWER 2 OF 2 BIOSIS COPYRIGHT (c) 2004 The Thomson Corporation. on STN
AN 1999:443060 BIOSIS
DN PREV199900443060
TI Three and **four dimensional**-quantitative structure activity relationship (3D/4D-QSAR) analyses of **CYP2D6** inhibitors.
AU **Ekins, Sean**; Bravi, Gianpaolo; Binkley, Shelly; Gillespie, Jennifer S.; Ring, Barbara J.; Wikel, James H.; Wrighton, Steven A. [Reprint author]
CS Department of Drug Disposition, Lilly Research Laboratories, Lilly Corporate Center, Eli Lilly and Co., Indianapolis, IN, 46285, USA
SO Pharmacogenetics, (Aug., 1999) Vol. 9, No. 4, pp. 477-489. print. ISSN: 0960-314X.
DT Article
LA English
ED Entered STN: 26 Oct 1999
Last Updated on STN: 26 Oct 1999
AB Three- and **four-dimensional** quantitative structure activity relationship (3D/4D-QSAR) pharmacophore models of competitive inhibitors of **CYP2D6** were constructed using data from our laboratory or the literature. The 3D-QSAR pharmacophore models of the common structural features of **CYP2D6** inhibitors were built using the program Catalyst(R) (Molecular Simulations, San Diego, CA, USA). These 3D-QSAR models were compared with 3D and 4D-QSAR partial least squares (PLS) models which were constructed using molecular surface-weighted holistic invariant molecular (MS-WHIM) descriptors of size and shape of inhibitors. The first Catalyst(R) model was generated from multiple conformers of competitive inhibitors (n = 20) of **CYP2D6** mediated bufurolol 1'-hydroxylation. This model demonstrated a correlation of observed and predicted Ki (apparent) values of r = 0.75. A second Catalyst(R) model was constructed from literature derived Ki (apparent) values (n = 31) for the inhibition of **CYP2D6**. This model provided a correlation of observed and predicted inhibition for **CYP2D6** of r = 0.91. Both Catalyst(R) Ki pharmacophores were then validated by predicting the Ki (apparent) of a test set of known **CYP2D6** inhibitors (n = 15). Ten out of 15 of these Ki (apparent) values were predicted to be within one log residual of the observed value using our **CYP2D6** inhibitor model, while the literature model predicted nine out of 15 values. Similarly, 3D- and 4D-QSARs derived from PLS MS-WHIM for our dataset yielded predictable models as assessed using cross-validation. The corresponding cross-validated PLS MS-WHIM model for the literature dataset yielded a comparable 3D-QSAR and improved 4D-QSAR value. Such computational models will aid in future prediction of drug-drug interactions.

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.01	6.22

STN INTERNATIONAL LOGOFF AT 11:13:24 ON 03 DEC 2004